

COMPONENTS:

- (1) Benzene; C₆H₆; [71-43-2]
 (2) Seawater

EVALUATOR:

D.G. Shaw
 Institute of Marine Science
 University of Alaska
 Fairbanks, Alaska USA

December 1982

CRITICAL EVALUATION:

The solubility of benzene (1) in seawater (2) at 298 K has been reported by the following workers:

<u>Authors</u>	<u>Method</u>	<u>Salinity</u> g salts/kg sln	<u>g(l)/100 g sln</u>
Mackay and Shiu (ref 2)	GLC	35	0.1340
Price (ref 3)	GLC	34.472	0.1391
May <i>et al.</i> (ref 4)	HPLC	35	0.1365

These three determinations made by two methods agree within their experimental error of 8 to 10%. Each group of workers has also determined the solubility of benzene in pure water and obtained results within the same error of the value recommended in this volume. Therefore, the mean of the reported values, 0.135 g(l)/100 g sln, is accepted as the recommended value at the indicated temperature and salinity. These studies measured solubility over a range of salinities. Mackay and Shiu and May *et al.* reported their data in terms of the Setschenow equation. Their values of K_s (0.1836 and 0.175 L/mol) indicate the same (within experimental error) dependence of solubility on salinity and may be used to interpolate solubilities at other salinities up to 200 g salts/kg sln.

Brown *et al.* (ref 1) determined the solubility of benzene in seawater at a salinity of 34.42 g salts/kg sln over the temperature range 273 to 293 K. Linear extrapolation by the evaluator of these results to 298 K gives a value of 0.127 g(l)/100 g sln. This suggests that the results of Brown *et al.* may be slightly low.

SOLUBILITY OF BENZENE (1) IN SEAWATER (2)
RECOMMENDED VALUE

<u>T/K</u>	<u>g salts/kg sln</u>	<u>g(l)/100 g sln</u>
298	35	0.136

Since the solubility of seawater (1) and benzene (2) has been reported only by Umamo and Hayano (ref 5), no critical evaluation is possible. The interested reader is referred to the relevant data sheet which is included with the preceding benzene-water system.

REFERENCES

- Brown, R.L.; Wasik, S.P.; *J. Res. Natl. Bur. Stds. A.* 1974, *78*, 453-60.
- Mackay, D.; Shiu, W.Y. *Can. J. Chem. Eng.* 1975, *53*, 239-42.
- Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.
- May, W.E.; Wasik, S.P.; Freeman, D.H. *Anal. Chem.* 1978, *50*, 997-1000.
- Umamo, S.; Hayano, I.; *Kogyo Kagaku Zasshi* 1957, *60*, 1436-7.

COMPONENTS: (1) Benzene; C ₆ H ₆ ; [71-42-2] (2) Artificial seawater	ORIGINAL MEASUREMENTS: Brown, R.L.; Wasik, S.P. <i>J. Res. Natl. Bur. Stds. A.</i> <u>1974</u> , 78, 453-60.
VARIABLES: Temperature: 0-20°C Salinity: 34.42 g salts/kg sln	PREPARED BY: G.T. Hefter and D.G. Shaw

EXPERIMENTAL VALUES:

Solubility of benzene in artificial seawater

$t/^\circ\text{C}$	$\text{g(l)}/100 \text{ g sln}^a$	$10^4 x_1$ (compiler)
0.19	0.1323 (0.0017)	3.129
5.32	0.1376 (0.0022)	3.255
10.05	0.1347 (0.0023)	3.186
14.96	0.1318 (0.0025)	3.117
20.04	0.1296 (0.0022)	3.065

^a numbers in parentheses are standard deviations from 4 observations

AUXILIARY INFORMATION**METHOD/APPARATUS/PROCEDURE:**

Solubilities were calculated from partition coefficient measurements for the hydrocarbon between an aqueous solution and its vapor using headspace chromatography.

The apparatus and the method of obtaining the partition coefficients are described in detail in the paper. The hydrocarbon was introduced as a vapor (to avoid emulsification) into a glass equilibration cell containing about 45 cm³ of water. The vapor was subsequently analysed by gas chromatography using He as the carrier. Possible sources of error are discussed in detail although the source of vapor pressure data used to calculate solubilities are not given.

SOURCE AND PURITY OF MATERIALS:

- (1) 99.99 mole per cent purity; source and methods of purification not specified.
- (2) Prepared according to ref. 1. Purity not specified.

ESTIMATED ERROR:

Temperature: ± 0.01 K

Solubility: see Table above

REFERENCES:

1. Sverdrup, H.U.; Johnson, M.W.; Fleming, R.H.; *The Oceans* 1942, Prentice-Hall, Englewood Cliffs, New Jersey p186.

COMPONENTS: (1) Benzene; C ₆ H ₆ ; [71-43-2] (2) Sodium chloride; NaCl; [7647-14-5] (3) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Mackay, D.; Shiu, W.Y. <i>Can. J. Chem. Eng.</i> 1975, 53, 239-42.
VARIABLES: One temperature: 25°C Salinity: 0-200 g(2)/kg sln	PREPARED BY: M. Kleinschmidt and W. Shiu
EXPERIMENTAL VALUES: The solubility of benzene in solutions of sodium chloride is reported in terms of the Setschenow equation: $\log(S_0/S) = K_s C_s$ where, S ₀ is the solubility of benzene in water (mg/L) S is the solubility of benzene in solution (mg/L) K _s is the Setschenow constant (L/mol) C _s is the concentration of sodium chloride (L/mol) evaluating the equation for S over the range of C _s 0-4 mol/L, K _s = 0.1836 ± 0.0072 (standard error) with S ₀ = 1779.5 ± 16.4. The corresponding mass percent and mole fraction, x ₁ , at salinity = 35 g(2)/kg sln calculated by the compilers are 0.1340 g(1)/100 g sln and 3.227 x 10 ⁻⁴ assuming a solution density of 1.025 kg/L.	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: Solubility was determined by vapor phase extraction and gas chromatographic analysis. This method does not require the preparation of saturated solutions and thus avoids one of the major sources of error of other methods.	SOURCE AND PURITY OF MATERIALS: (1) research grade, 99.9+%, from Phillips Petroleum Co. (2) and (3) not specified ESTIMATED ERROR: temp. ± 0.1 K soly. 95% confidence limit is about 8% REFERENCES:

COMPONENTS: (1) Benzene; C ₆ H ₆ ; [71-43-2] (2) Sodium chloride; NaCl; [7647-14-5] (3) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Price, L.C. <i>Am. Assoc. Petrol. Geol. Bull.</i> <u>1976</u> , 60, 213-44.
---	--

VARIABLES: One temperature: 25°C Salinity: 1-360 g(2)/kg sln	PREPARED BY: M. Kleinschmidt and D. Shaw
---	--

EXPERIMENTAL VALUES:

Solubility of Benzene in Aqueous NaCl

Salinity g(2)/kg sln	Mass Percent g(1)/100 g sln	Mole fraction 10 ⁴ x ₁ (compilers)
1.002	0.1718	3.96
10.000	0.1628	3.78
34.472 ^a	0.1391	3.28
50.030	0.1194	2.85
125.100	0.0593	1.48
199.900	0.0388	1.01
279.800	0.0214	0.581
358.700	0.0134	0.378

^aArtificial seawater, composition not specified but probably similar to ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: Details given in source. (1) was equilibrated with NaCl solution for one month. An aliquot was analyzed directly by gas chromatography.	SOURCE AND PURITY OF MATERIALS: (1) commercial, 99 + % pure
	ESTIMATED ERROR: Temperature ± 1 K Solubility ± 10 relative % REFERENCES: 1. Lyman, J.; Fleming, R.H.; <i>J. Mar. Res.</i> <u>1940</u> , 3, 135.

COMPONENTS: (1) Benzene; C_6H_6 ; [71-43-2] (2) Sodium Chloride; NaCl; [7647-14-5] (3) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: May, W.E.; Wasik, S.P.; Freeman D.H. <i>Anal. Chem.</i> <u>1978</u> , 50, 997-1000.
VARIABLES: One temperature: 25°C Salinity: 0-40 g(2)/kg sln	PREPARED BY: W.Y. Shiu and D. Mackay
EXPERIMENTAL VALUES: <p>The solubility of benzene in aqueous sodium chloride is reported in terms of the Setschenow equation:</p> $\log(S_0/S) = K_s C_s$ <p>where;</p> <p>S_0 is the solubility of (1) in water (mg/L) S is the solubility of (1) in saline solution (mg/L) K_s is the Setschenow constant (L/mol) C_s is the concentration of sodium chloride (mol/L)</p> <p>evaluating the equation for S over the range of C_s 0-0.7 mol/L, $K_s = 0.175$ with $S_0 = 1791$.</p> <p>The corresponding mass percent and mole fraction x_1, at salinity = 35 g(2)/kg sln calculated by the compilers are 0.1365 g(1)/100 g sln and 3.22×10^{-4}.</p>	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: A saturated solution of (1) was prepared by pumping salt water through a "generation column" which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an "extractor column" packed with a superficially porous bonded C_{18} stationary phase, then a water-acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.	SOURCE AND PURITY OF MATERIALS: (1) greater than 97% pure. (2) reagent grade. (3) distilled from potassium permanganate-sodium hydroxide and passed through an XAD-2 column. ESTIMATED ERROR: temp \pm 0.05 K $K_s \pm$ 0.006 $S_0 \pm$ 10
	REFERENCES: